CUQM-119, HEPHY-PUB 822/06
math-ph/0702047

Schrödinger secant lower bounds to semirelativistic eigenvalues

Richard L. Hall[1] and Wolfgang Lucha[2]

[1] *Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve Boulevard West, Montréal, Québec, Canada H3G 1M8*
E-mail: rhall@mathstat.concordia.ca

[2] *Institute for High Energy Physics, Austrian Academy of Sciences, Nikolsdorfergasse 18, A-1050 Vienna, Austria*
E-mail: wolfgang.lucha@oeaw.ac.at

Abstract

It is shown that the ground-state eigenvalue of a semirelativistic Hamiltonian of the form $H = \sqrt{m^2 + p^2} + V$ is bounded below by the Schrödinger operator $m + \beta p^2 + V$, for suitable $\beta > 0$. An example is discussed.

Key words: Semirelativistic Hamiltonians,Salpeter Hamiltonians, Schrödinger lower bound, secant lower bound

1 Introduction

We study semirelativistic Hamiltonians H composed of the relativistically correct expression $K(p^2) = \sqrt{m^2 + p^2}$, $p \equiv |\mathbf{p}|$, for the energy of a free particle of mass m and momentum $\mathbf{p}$, and of a coordinate-dependent static interaction potential $V(r)$, $r \equiv |\mathbf{r}|$, which may be chosen arbitrarily, apart from the constraint imposed on H that it be bounded from below:

$$H = \sqrt{m^2 + p^2} + V(r). \tag{1.1}$$

The eigenvalue equation generated by this kind of Hamiltonian is usually called the spinless Salpeter equation. It arises as a well-defined approximation to the Bethe–Salpeter formalism for the description of bound states within (relativistic) quantum field theory [1] when it is assumed that the bound-state

constituents interact instantaneously and propagate like free particles [2]. At the same time, H may be regarded as the simplest and perhaps most straightforward generalization of a (nonrelativistic) Schrödinger operator towards the incorporation of relativistic kinematics. For many potentials, this Hamiltonian can be shown [3] to be bounded below and essentially self-adjoint, and its spectrum can be defined variationally. For definiteness, we consider the corresponding eigenvalue problem in three spatial dimensions.

2 The secant lower bound

The kinetic-energy operator $K = \sqrt{m^2 + p^2}$ is a concave function of the Schrödinger kinetic energy p^2. Hence, tangential operators to K of the form $\alpha + \beta p^2$ provide a class of Schrödinger upper bounds to K. This idea has been explored and optimized in earlier papers [4,5,6,7]. In the present paper we are concerned with lower bounds. The question arises as to whether any of the family of Schrödinger operators $\alpha + \beta p^2 + V$ might generate a lower bound to H. On the basis of the usual comparison theorem of quantum mechanics one would not expect this since (in momentum space) the graph of $\alpha + \beta k^2$ either lies above K or crosses K. However, under suitable conditions, the comparison theorem has been strengthened [8] to yield spectral inequalities even when the corresponding potential graphs cross over. For our problem, we must compare the two Hamiltonians $H = K + V$ and $H^{(s)} = m + \beta p^2 + V$, where $\alpha = m$ and $\beta > 0$ is not yet chosen; $V(r)$ is assumed to be a spherically symmetric attractive potential in three spatial dimensions. Let us suppose that the exact normalized ground state of H is $\psi(r)$ and the corresponding momentum-space function is $\phi(k)$: these are normalized 'radial' functions including a factor r or k and satisfying, for example, $\psi(0) = 0$, $\int_0^\infty \psi^2(r)dr = 1$, and

$$\phi(k) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty \sin(kr)\psi(r)dr. \tag{2.1}$$

Similarly, for the Schrödinger comparison operator $H^{(s)}$, the wave functions are $\psi^{(s)}(r)$ and $\phi^{(s)}(k)$. Following the same reasoning as with two different potentials, which we used in the proof of Theorem 3 in Ref. [8], we consider the two eigenequations in momentum space (where V now becomes the integral operator $\tilde{V}$):

$$\left(\sqrt{m^2 + k^2} + \tilde{V}\right)\phi = E\phi, \tag{2.2}$$

$$\left(m + \beta k^2 + \tilde{V}\right)\phi^{(s)} = E^{(s)}\phi^{(s)}. \tag{2.3}$$

If we multiply (2.2) by $\phi^{(s)}$ and (2.3) by ϕ, subtract, and integrate on $[0,\infty)$, we obtain

$$I = \int_0^\infty \left(\sqrt{m^2+k^2} - (m+\beta k^2)\right)\phi(k)\phi^{(s)}(k)dk = \left(E - E^{(s)}\right)\int_0^\infty \phi(k)\phi^{(s)}(k)dk. \tag{2.4}$$

Now we proceed to declare our assumptions and to choose β. We first define the function $W(k)$ as follows

$$W(k) = \int_0^k \left(\sqrt{m^2+t^2} - (m+\beta t^2)\right)\phi^{(s)}(t)tdt. \tag{2.5}$$

The integral I on the left-hand side of (2.4) may then be integrated by parts to yield

$$I = -\int_0^\infty W(k)\left(\frac{\phi(k)}{k}\right)' dk. \tag{2.6}$$

We now show that $I \geq 0$ and that this in turn proves that $E^{(s)} \leq E$. To this end we make some assumptions concerning the two wave functions: (1) we assume that $\phi^{(s)}(k) \geq 0$ and (2) that $\phi(k) \geq 0$ and also $(\phi(k)/k)' \leq 0$. That is to say, we assume that the two wave functions are node free, and that the wave function for the semirelativistic problem (with the factor k removed) is monotone non-increasing. These assumptions have to be considered for each application. The final step is to choose β so that $I \geq 0$. This is achieved by the requirement that $W(\infty) = 0$. Clearly this determines β. Moreover, the graphs of $\sqrt{m^2+k^2}$ and $m + \beta k^2$, which are shown in Fig. 1, cross exactly twice, at $k = 0$, after which K is immediately larger than the Schrödinger operator, until they cross again. Meanwhile the integral of the difference up to infinity is zero. Thus we conclude $W(k) \geq 0$. This combined with the assumed positivity and monotonicity of $\phi(k)/k$ guarantees both that $I \geq 0$ and that the integral on the right-hand side of (2.4) is positive. Consequently, we have established the secant lower bound, $E^{(s)} \leq E$. This completes the simple proof.

For nonrelativistic problems curious examples have been constructed [9] in which there are arbitrarily large numbers of potential cross overs, but spectral ordering is still guaranteed.

A natural application to consider would be the Coulomb problem $V(r) = -c/r$, with coupling not too large, that is, $c < 2/\pi$. However, the integral in (2.5) is not defined for this problem since the momentum-space expression of the exact Schrödinger radial function is of the form $\phi^{(s)}(k) = Ak(a^2+k^2)^{-2}$, and one term also includes the factor k^3. In the next section we consider the example of the harmonic oscillator in some detail; here there is no such difficulty since the momentum-space Schrödinger wave function is Gaussian.

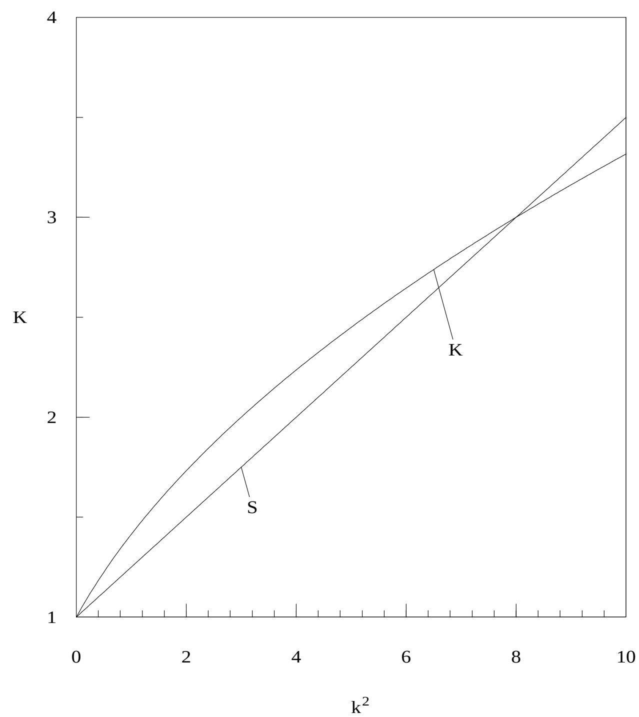

Fig. 1. Plot of semirelativistic $K = \sqrt{m^2 + k^2}$ and Schrödinger $S = m + \beta k^2$ kinetic-energy functions against k^2 in non-dimensional units with $m = 1$. The value $\beta = 0.2506$ is chosen so that $W(\infty) = 0$ for $V(r) = r^2$, which implies $W(k) \geq 0,\ k \geq 0$.

3 An example

We now consider a test example for which there are known (numerically) exact results. The harmonic oscillator is equivalent to a nonrelativistic problem whose spectrum can be determined numerically to high accuracy. Thus we have

$$\sqrt{m^2 + p^2} + r^2 \equiv p^2 + \sqrt{m^2 + r^2} \to \epsilon_2(m), \tag{3.1}$$

where $\epsilon_2(m)$ is the ground-state energy of the semirelativistic oscillator in three dimensions. Elementary scaling arguments then allow us to write more generally, with coupling $c > 0$, that

$$\sqrt{m^2 + p^2} + cr^2 \equiv cp^2 + \sqrt{m^2 + r^2} \to c^{\frac{1}{3}}\epsilon_2(mc^{-\frac{1}{3}}). \tag{3.2}$$

According to our present theory, a lower bound for this problem is given by the Schrödinger operator $H^{(s)} = m + \beta p^2 + cr^2$, with exact momentum-space eigenfunction $\phi^{(s)}(k)$. We must first be sure that the unknown exact

momentum-space wave function $\phi(k)$ is node free, and that $\phi(k)/k$ is monotone non-increasing. For well-behaved potentials, the ground state is generally node free [3]. We know that the second condition is also satisfied because of the following argument. In momentum space the eigenequation for the semirelativistic problem may be written

$$-c\phi''(k) + \sqrt{m^2+k^2}\ \phi(k) = E\phi(k). \tag{3.3}$$

The potential function $\sqrt{k^2+m^2}$ is bounded below and is monotone increasing. Hence, by the result proved at the start of Sec. 4 of Ref. [8], we know that the function $\phi(k)/k$ is indeed monotone non-increasing. We must now choose β to satisfy $W(\infty)=0$, that is to say

$$\int\limits_0^\infty \left(\sqrt{m^2+k^2} - \left(m+\beta k^2\right)\right) \exp\left(-\tfrac{1}{2}k^2(\beta/c)^{\frac{1}{2}}\right) k^2 dk = 0. \tag{3.4}$$

After a change of variables and some elementary Gaussian integrals, this condition may be written

$$g\left(\gamma^2\right) = \frac{\sqrt{\pi}}{2}\left(\gamma + \frac{3m\beta}{2\gamma}\right), \tag{3.5}$$

where the function g and the parameter γ are defined by

$$g(x) = \int\limits_{-\infty}^{\infty} \left(x+t^2\right)^{\frac{1}{2}} e^{-t^2}t^2 dt \quad \text{and} \quad \gamma = \left(\frac{m^4\beta}{4c}\right)^{\frac{1}{4}}. \tag{3.6}$$

Thus, for each choice of coupling $c>0$, the recipe for the lower bound may be written

$$m^3 = \frac{6c\gamma^2}{\left(\frac{2}{\gamma\sqrt{\pi}}\right) g(\gamma^2) - 1} \to \boxed{\gamma}, \quad \beta = \frac{4c\gamma^4}{m^4}, \quad E^L = m + 3\left(\beta c\right)^{\frac{1}{2}}. \tag{3.7}$$

By taking the case $c=1$ and using these formulae, we find the results shown in Table 1.

It is consistent with elementary physical arguments, and, indeed, with the Schrödinger upper bounds discussed earlier [5], that the Schrödinger lower bounds presented here also show that the semirelativistic problem becomes less relativistic as m increases; in the limit $m\to\infty$, both upper and lower bounds approach the asymptotic form

$$E \to m + 3\sqrt{\frac{c}{2m}}.$$

Similar results are obtained for the linear potential $V(r)=r$. In this case we have $\psi^{(s)}(r) = C\mathrm{Ai}(r\beta^{-\frac{1}{3}} - e_1)$, Where Ai is the Airy function, and $e_1 \approx$

Table 1
The secant lower bound $E^{(s)}$ and corresponding accurate ground-state eigenvalues E for the problem $H = \sqrt{m^2 + p^2} + r^2$ in R^3. The values of β are shown, which guarantee that the Schrödinger operator $H^{(s)} = m + \beta p^2 + r^2$, whose lowest energy is $E^{(s)}$, indeed provides a lower bound.

m	β	$E^{(s)}$	E
0.1	0.4034	2.0055	2.3422
0.2	0.3788	2.0464	2.3544
0.5	0.3190	2.1943	2.4323
1	0.2506	2.5019	2.6640
2	0.1734	3.2492	3.3361
3	0.1315	4.0880	4.1415
4	0.1056	4.9747	5.0105
5	0.0879	5.8897	5.9153
7	0.0657	7.7692	7.7840
10	0.0475	10.6539	10.6619

2.33811 is the bottom of the spectrum of $p^2 + r$. For $m = 2\sqrt{2}$, for example, we find $\beta = 0.13272$ and $E \geq 4.021$, whereas an accurate numerical value [10] is $E = 4.080$.

4 Conclusion

Because of the concavity of the semirelativistic Hamiltonian $H = \sqrt{m^2 + p^2} + V(r)$ in p^2, it would seem unlikely at first glance that one could find lower bounds to the energy based on Schrödinger comparison operators. In spite of this expectation, we show in this paper that such a lower bound is possible. The secant bound involves a comparison operator whose kinetic-energy function $m + \beta p^2$ has a graph which crosses that of the semirelativistic expression $K = \sqrt{m^2 + p^2}$.

Acknowledgements

Partial financial support of this work under Grant No. GP3438 from the Natural Sciences and Engineering Research Council of Canada, and the hospitality of the Institute for High Energy Physics of the Austrian Academy of Sciences in Vienna, are gratefully acknowledged by one of us [RLH].

References

[1] E. E. Salpeter and H. A. Bethe, Phys. Rev. **84**, 1232 (1951).

[2] E. E. Salpeter, Phys. Rev. **87**, 328 (1952).

[3] E. H. Lieb and M. Loss, *Analysis* (American Mathematical Society, New York, 1996). The definition of the Salpeter kinetic-energy operator is given on p. 168.

[4] R. L. Hall, W. Lucha, and F. F. Schöberl, Int. J. Mod. Phys. A **17**, 1931 (2002).

[5] R. L. Hall, W. Lucha, and F. F. Schöberl, J. Math. Phys. **43**, 5913 (2002).

[6] R. L. Hall, W. Lucha, and F. F. Schöberl, J. Math. Phys. **45**, 3086 (2004).

[7] R. L. Hall and W. Lucha, J. Phys. A **38**, 7997 (2005).

[8] R. L. Hall, J. Phys. A **25**, 4459 (1992).

[9] R. L. Hall and N. Saad, Phys. Lett. A **237**, 107 (1998).

[10] S. Boukraa and J.-L. Basdevant, J. Math. Phys. **30**, 1060 (1989).